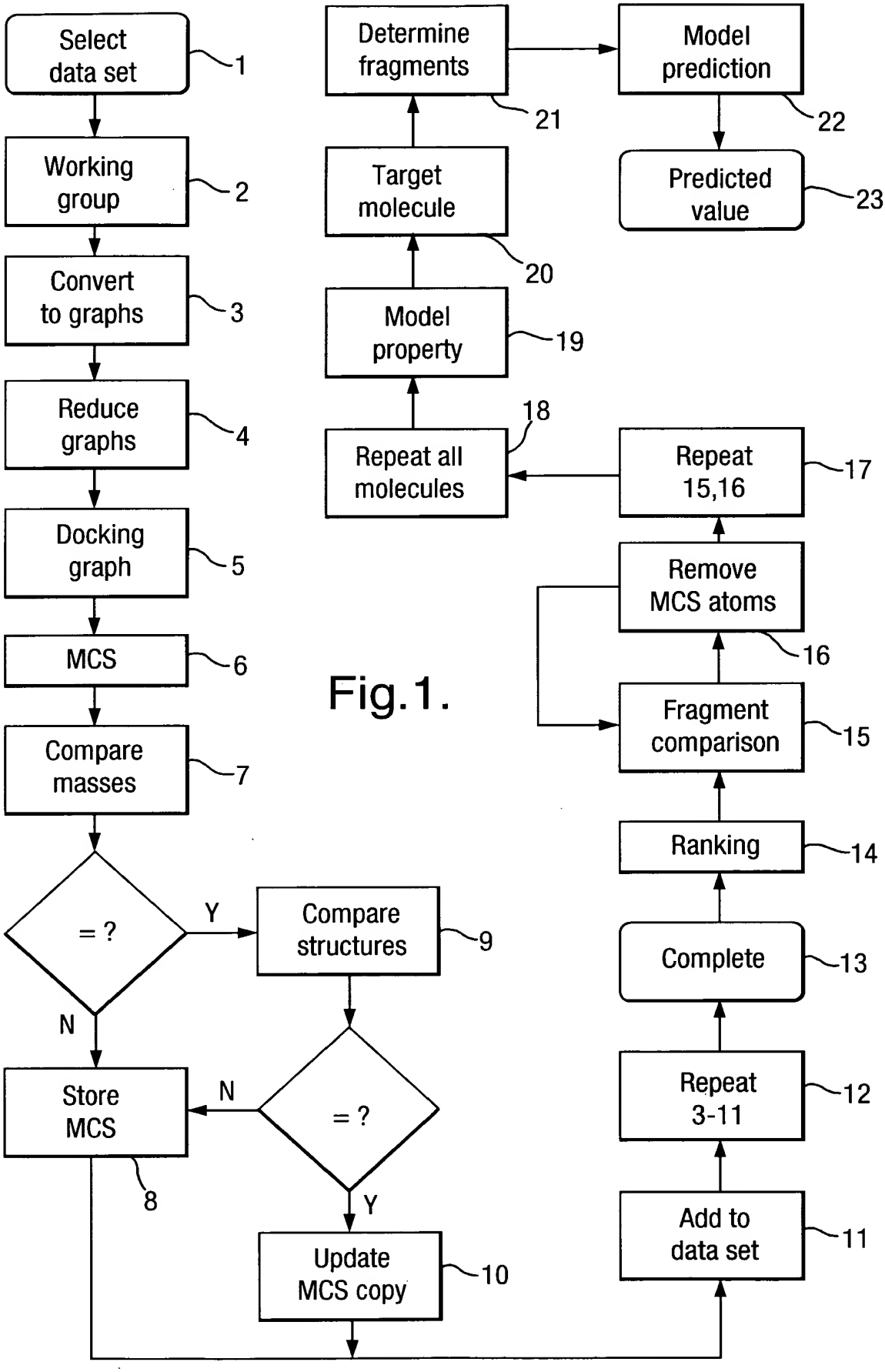

Select data set
1
Working group
2
Convert to graphs
3
Reduce graphs
4
Docking graph
5
MCS
6
Compare masses
7
= ?
Y
N
Compare structures
9
= ?
N
Y
Store MCS
8
Update MCS copy
10
Add to data set
11
Repeat 3-11
12
Complete
13
Ranking
14
Fragment comparison
15
Remove MCS atoms
16
Repeat 15,16
17
Repeat all molecules
18
Model property
19
Target molecule
20
Determine fragments
21
Model prediction
22
Predicted value
23

Fig.1.

Fig.2.

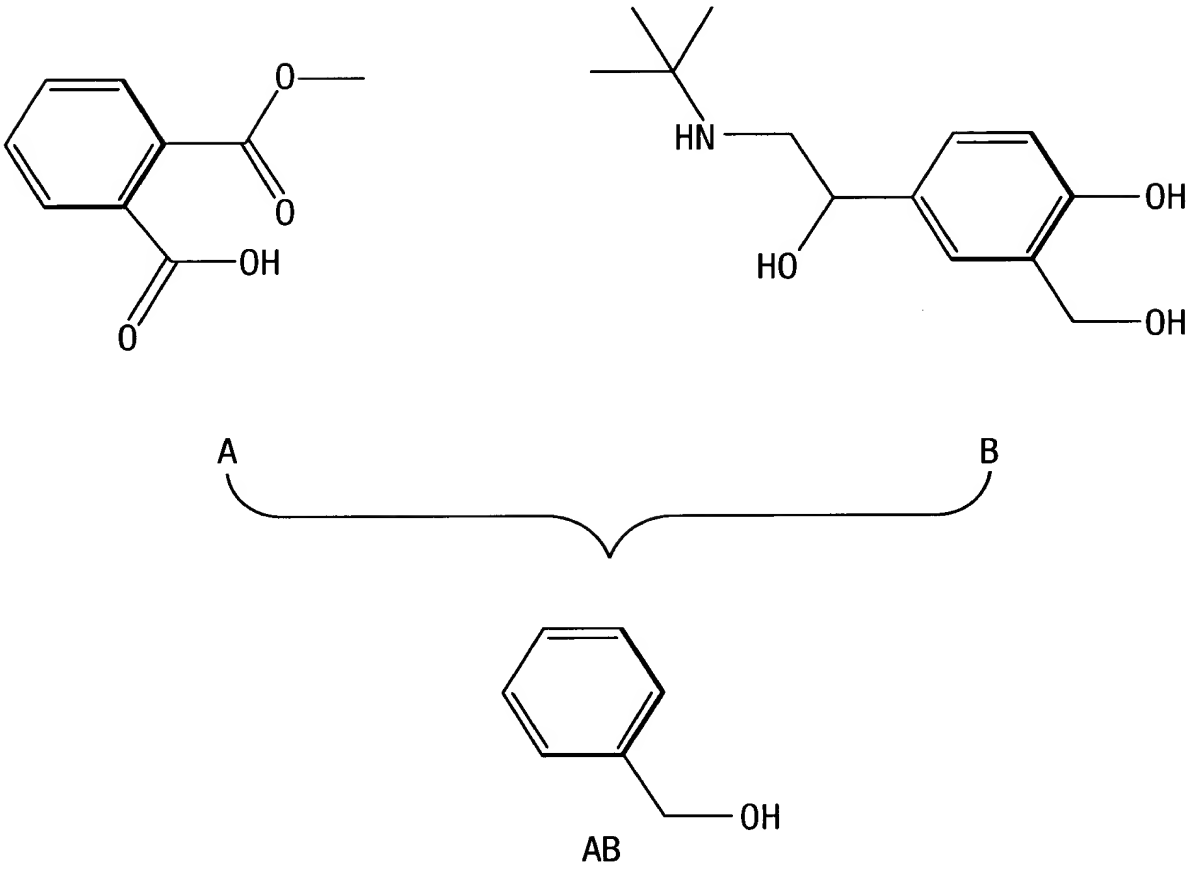


Fig.3.

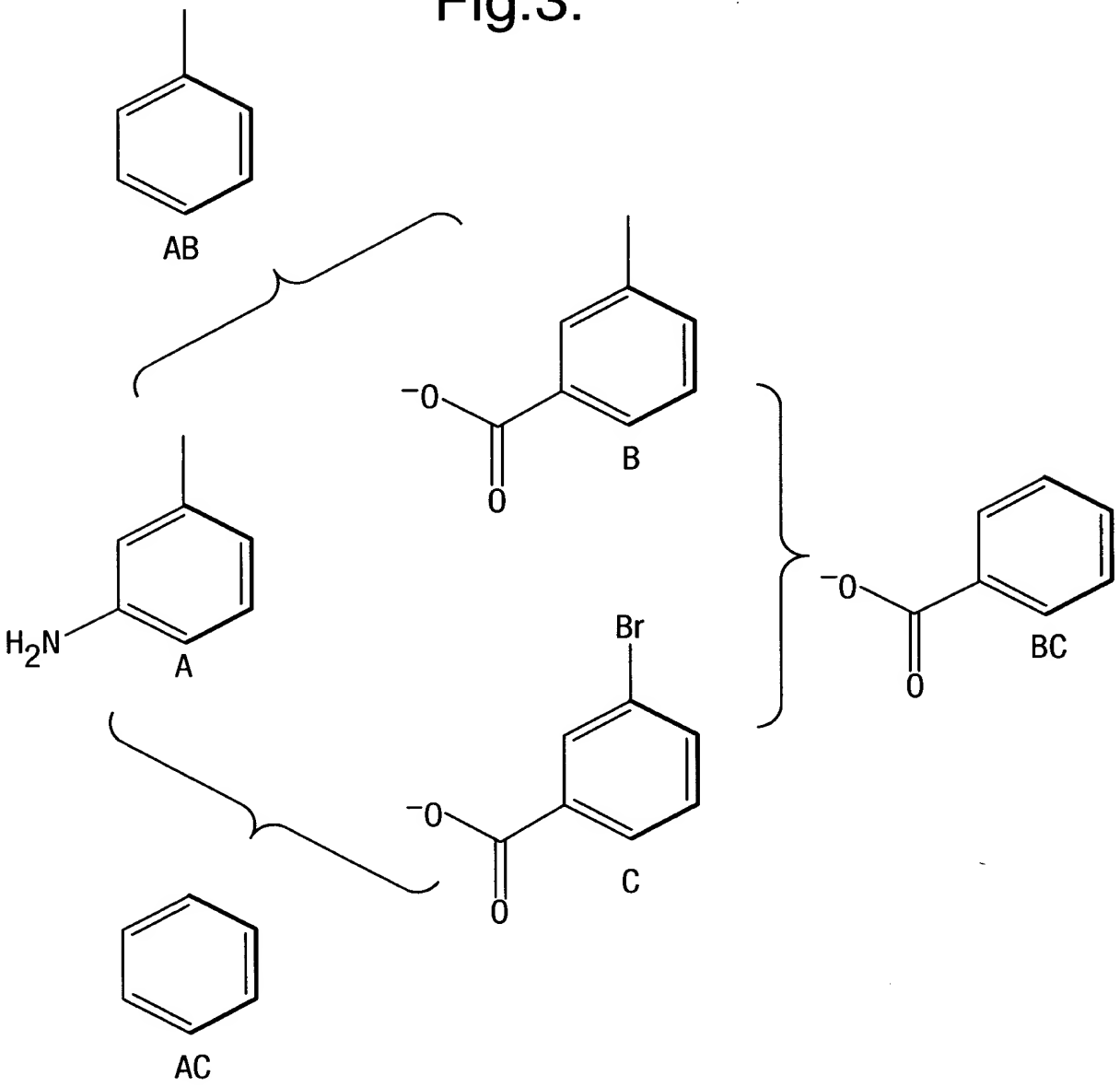
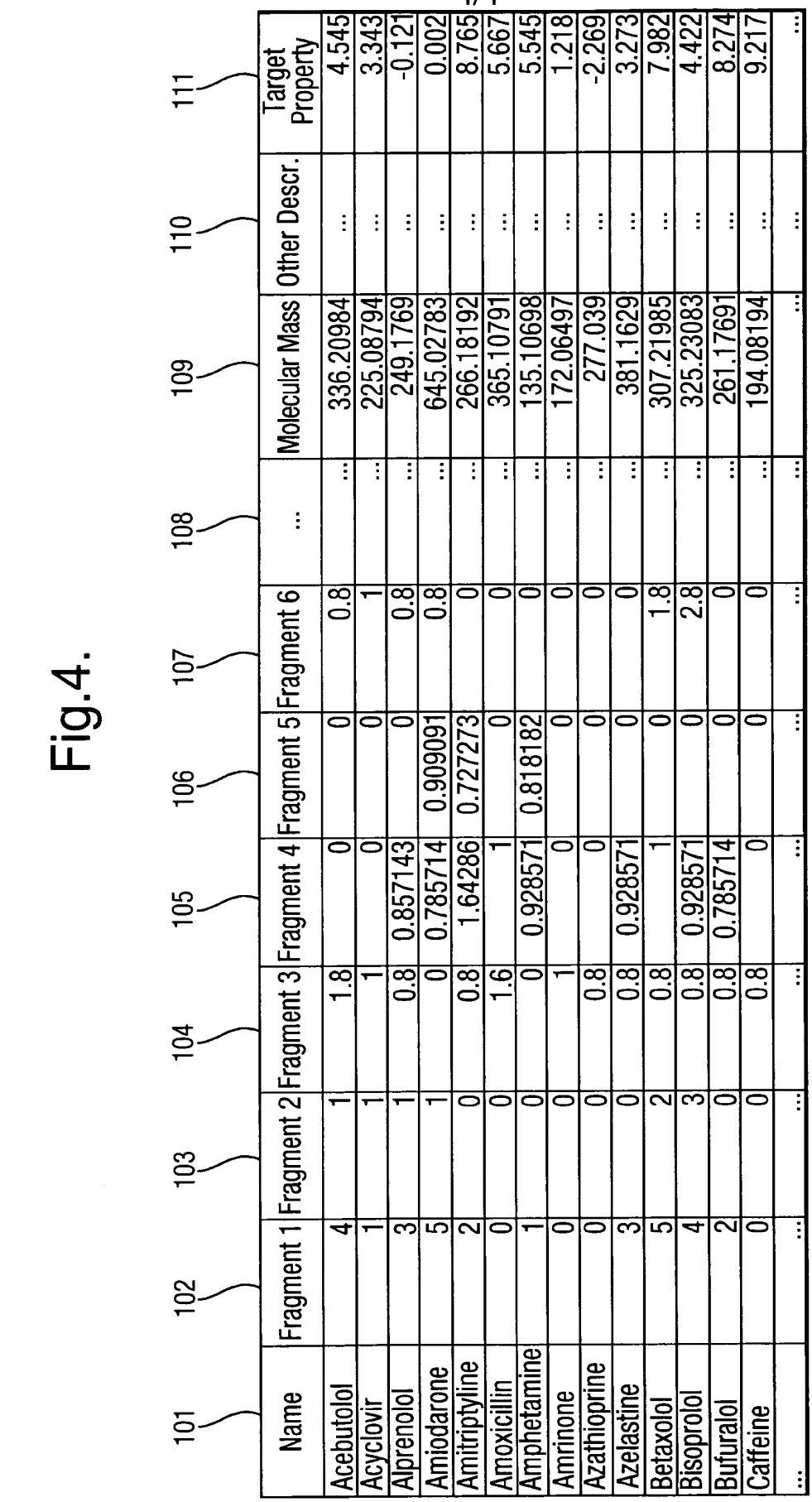


Fig.4.



101 Name	102 Fragment 1	103 Fragment 2	104 Fragment 3	105 Fragment 4	106 Fragment 5	107 Fragment 6	108 ...	109 Molecular Mass	110 Other Descr.	111 Target Property
Acebutolol	4	1	1.8	0	0	0.8	...	336.20984	...	4.545
Acyclovir	1	1	1	0	0	1	...	225.08794	...	3.343
Alprenolol	3	1	0.8	0.857143	0	0.8	...	249.1769	...	-0.121
Amiodarone	5	1	0	0.785714	0.909091	0.8	...	645.02783	...	0.002
Amitriptyline	2	0	0.8	1.64286	0.727273	0	...	266.18192	...	8.765
Amoxicillin	0	0	1.6	1	0	0	...	365.10791	...	5.667
Amphetamine	1	0	0	0.928571	0.818182	0	...	135.10698	...	5.545
Amrinone	0	0	1	0	0	0	...	172.06497	...	1.218
Azathioprine	0	0	0.8	0	0	0	...	277.039	...	-2.269
Azelastine	3	0	0.8	0.928571	0	0	...	381.1629	...	3.273
Betaxolol	5	2	0.8	1	0	1.8	...	307.21985	...	7.982
Bisoprolol	4	3	0.8	0.928571	0	2.8	...	325.23083	...	4.422
Bufuralol	2	0	0.8	0.785714	0	0	...	261.17691	...	8.274
Caffeine	0	0	0.8	0	0	0	...	194.08194	...	9.217
...	...	...	...	...	...	...	...	...	...	...